Computation of the Nonlinear Magnetic Response of a Three Dimensional Anisotropic Superconductor

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Many problems in computational magnetics involve computation of fields which decay within a skin depth δ, much smaller than the sample size d. We discuss here a novel perturbation method which exploits the smallness of $\epsilon \equiv \delta/d$ and the asymptotic behavior of the solution in the exterior and interior of a sample. To illustrate this procedure we consider the computation of the magnetic dipole and quadrupole moments of an anisotropic, unconventional, three dimensional superconductor. The method significantly reduces the required numerical work and can be implemented in different numerical algorithms.

I. INTRODUCTION

In various problems of electrodynamics, field penetration is characterized by a skin depth, δ, much smaller than the actual sample size, d. For many purposes, the approximation of zero skin depth, or that eddy currents flow only as surface sheet currents, is not sufficiently accurate, as a detailed knowledge of the field penetration or accurate values of magnetic multipoles are required. It is then important to include the small corrections arising from finite skin depth.

In this paper we examine the inclusion of skin depth corrections, focusing on the magnetic response of a high temperature superconductor (HTSC). For HTSC's, it is known[1−3] that examining the field penetration yields important information about the unconventional electronic pairing states in these materials and the still unknown nature of high temperature superconductivity.

Although we focus on this problem, our ideas have broad validity and applications. The magnetic response of a superconductor is related to that of an ordinary conductor in an harmonically applied field. The skin effect, with $\delta \ll d$, for a quasi-static regime where the frequency is restricted by $\omega \ll c/d$ (c is the speed of light), maps[4] onto the problem of a superconductor of the same size and shape in a static applied magnetic field. The role of δ for a conductor is taken up by λ, the effective penetration depth of a superconductor ($\lambda \ll d$). Except for the simplest geometries where an analytic solution exists for the corresponding boundary value problem, obtaining small skin depth corrections can be computationally demanding. These difficulties arise from the nontrivial boundary conditions (including open boundary equations at infinity) and the requirement that the appropriate, generally nonlinear differential equations be solved very accurately within the narrow region where the skin effects are contained. Our method offers a way to resolve these difficulties.

We examine a superconductor in an applied uniform magnetic field, $\mathbf{H}_a$. The sample occupies a bounded region $\Omega \subset \mathbf{R}^3$ and at its boundary, $\partial\Omega$, is surrounded by vacuum. For H_a smaller than a critical value, a superconductor is in the Meissner regime: The magnetic flux is expelled from the bulk of the sample. On $\mathbf{R}^3 \backslash \Omega$ the current is $\mathbf{j} \equiv 0$ and it is sufficient to find a magnetic scalar potential Φ, $\mathbf{H} = -\nabla\Phi$, which satisfies the Laplace equation. On Ω, the appropriate Maxwell equation is Ampère's law. For unconventional pairing states in HTSC's, the London relation[5] $\mathbf{j} = \mathbf{j}(\mathbf{A})$ between current and vector potential[6] $\mathbf{A}$, is nonlinear and nonanalytic.[1,2,7] Thus it is advantageous to combine Ampère's law in terms of the vector potential with the relation $\mathbf{j}(\mathbf{A})$:

$$\nabla \times \nabla \times \mathbf{A} = \frac{4\pi}{c}\mathbf{j}(\mathbf{A}). \tag{1}$$

HTSC's in general have a highly anisotropic structure with different penetration depths, λ_i, along the various, $i = a, b, c$ crystallographic directions. We include this penetration depth anisotropy through the anisotropic, nonlinear, relation $\mathbf{j}(\mathbf{A})$ given in Ref. 7. By λ we shall denote the effective penetration depth (a function of λ_i), which plays the dominant role in the field decay studied. In the special case of an isotropic superconductor with a linear relation $\mathbf{j}(\mathbf{A})$, all the fields on Ω satisfy the vector Helmholtz equation $\nabla^2\mathbf{F} = \mathbf{F}/\lambda^2$, where $\mathbf{F}$ can be $\mathbf{H}$, $\mathbf{j}$, $\mathbf{A}$. The boundary conditions are: $-\nabla\Phi = \mathbf{H}_a$, at infinity, while on $\partial\Omega$ $\mathbf{H}$ is continuous[5] and there is no normal component of current, $j_n|_{\partial\Omega} = 0$. From the open boundary condition at infinity combined with the the continuity requirement it appears that to obtain the finite skin depth corrections, one would have to solve numerically the appropriate equations in all space.

II. PERTURBATION METHOD

To resolve these difficulties, we view the finite skin effects, i.e., for finite λ in a superconductor, as a small correction to the dominant perfect diamagnetic response at $\lambda = 0$. When skin effects are studied, one has to include these corrections, which are characterized by the small parameter $\epsilon \equiv \lambda/d \ll 1$. The boundary value problem in the $\epsilon = 0$ limit is relatively simple, one has only to solve

the Laplace equation for the scalar potential on $\mathbf{R}^3 \setminus \Omega$ with trivial Neumann boundary conditions on $\partial\Omega$. We assume that an accurate, either analytical or numerical, solution on $\mathbf{R}^3 \setminus \Omega$ in the $\epsilon = 0$ limit is available.[7] This will be the starting point from which we shall develop our perturbation method. The small skin effect is then treated as a perturbation from the $\epsilon = 0$ solution.

To proceed with the perturbation calculation we consider the auxiliary problem consisting of Eq. (1) on Ω, the $\epsilon = 0$ solution on $\mathbf{R}^3 \setminus \Omega$, and the boundary conditions on $\partial\Omega$, $j_n = 0$ and continuity of the tangential component of $\mathbf{H}$ (the continuity of H_n can not be imposed, it vanishes for the external fields in the $\epsilon = 0$ limit). This is computationally simple, as it decouples the solutions for the regions $\mathbf{R}^3 \setminus \Omega$ and Ω. From this auxiliary problem we can generate[7] the skin corrections to leading order in ϵ, as we shall now see.

In this paper we consider the magnetic moment of a superconductor for an arbitrary direction of $\mathbf{H}_a$ in a sample without a rotational symmetry (this is an extension of Ref. 7), and the magnetic quadrupole moment. We match the asymptotic behavior of the solution on $\mathbf{R}^3 \setminus \Omega$ and that in Ω by employing integral identities for magnetic multipoles.[7] At large distances from Ω, the multipole expansion of the fields can be considered and the asymptotic behavior is governed primarily by the lowest nonvanishing multipole term. There are two different ways to obtain the multipole moments: by examining the asymptotic behavior on $\mathbf{R}^3 \setminus \Omega$, and from the fields computed on Ω. By matching the asymptotic behavior we mean that the exact solution on $\mathbf{R}^3 \setminus \Omega$ is formally written in terms of the unknown multipole moments which must agree with those computed from the fields on Ω. We formulate integral identities to compute the magnetic multipoles from fields on Ω such that we can identify terms in these expressions which are of different orders in ϵ.

The magnetic moment[8] is

$$\mathbf{m} = \frac{1}{2c} \int_{\Omega} d\Omega \, \mathbf{r}'' \times \mathbf{j}(\mathbf{r}''), \tag{2}$$

where $\mathbf{r}''$ is the position vector for a point in Ω and $\mathbf{j}$ is found from Eq. (1). The components of $\mathbf{m}$ can be written for $\epsilon \ll 1$ in the form $m_i = m_{0i}(1 - \alpha_i \, \epsilon + O(\epsilon^2))$, $i = x, y, z$, where m_{0i}, denoting the $i-th$ component of the magnetic moment in the limit $\epsilon = 0$, represents a perfect diamagnetic response. For an ellipsoid it is given by a demagnetization factor. The α_i describe small corrections to perfect diamagnetism due to current penetration. For a direction i, where $m_{0i} = 0$ (it could vanish from symmetry arguments, for a particular direction of H_a), one can still have $\alpha_i \neq 0$, because of the anisotropic and nonlinear relation $\mathbf{j}(\mathbf{A})$. The effects of nonlinearity $\mathbf{j}(\mathbf{A})$, absent for $\epsilon = 0$, are typically small and can be thought of as field dependent corrections to α_i, linear in H_a.

To distinguish terms in Eq. (2) of various orders in ϵ, we use Ampère's law, identities from vector calculus, and Gauss' theorem to obtain[7]

$$\mathbf{m} = \frac{1}{8\pi} \int_{\partial\Omega} dS \, [\mathbf{n} \, (\mathbf{r}'' \cdot \mathbf{H}) + \, \mathbf{n} \times (\mathbf{r}'' \times \mathbf{H})] \\ + \frac{1}{8\pi} \int_{\Omega} d\Omega \, \mathbf{H} \equiv \mathbf{m}_1 + \mathbf{m}_2, \tag{3}$$

where $\mathbf{r}''$ is the position vector for a point on $\partial\Omega$ and $\mathbf{n}$ is the unit normal pointing outwards. The terms $\mathbf{m_1}$ and $\mathbf{m}_2$ are of different order in ϵ and the latter is small, i.e. of $O(\epsilon m_0)$. This can be seen from the expression for $\mathbf{m}_2$. Since $\mathbf{H}$ is confined to a "skin" layer of thickness λ, the integral over the whole volume of Ω is effectively only an integration over the region $\sim \lambda$ away from its surface. Thus $\mathbf{m}_2$ vanishes in the zero penetration limit ($\epsilon = 0$) and $\mathbf{m}(\epsilon = 0) \equiv \mathbf{m}_0 = \mathbf{m}_1$. In order to obtain $\mathbf{m}$ to $O(\epsilon m_0)$ it is sufficient to compute $\mathbf{m_2}$ to leading (zeroth) order. The term $\mathbf{m_2}$ explicitly scales with ϵ and any first order corrections for the fields needed to compute it would only produce contributions of order $O(\epsilon^2 m_0)$.

A similar integral identity can be derived for the magnetic quadrupole moment, defined[9] as a symmetric traceless tensor with components

$$Q_{ij} = \frac{1}{2c} \int_{\Omega} d\Omega \, [\mathbf{r}''(\mathbf{r}'' \times \mathbf{j}) + \mathbf{r}''[(\mathbf{r}'' \times \mathbf{j})]_{ij}, \;\; i, j = x, y, z. \tag{4}$$

Using the previously introduced notation for terms of different order in ϵ, $Q_{ij} \equiv Q_{1ij} + Q_{2ij}$ we can derive, employing integration by parts and standard identities:

$$Q_{1ij} = \frac{1}{8\pi} \int_{\partial\Omega} dS \, [[n_i r''_j + n_j r''_i] \, (\mathbf{r}'' \cdot \mathbf{H}) \\ - \; [r''_i H_j + r''_j H_i](\mathbf{n} \cdot \mathbf{r}'')], \tag{5a}$$

$$Q_{2ij} = \frac{1}{8\pi} \int_{\Omega} d\Omega \, [3 \, [r''_i H_j + r''_j H_i] - 2\delta_{ij}(\mathbf{r}'' \cdot \mathbf{H})], \tag{5b}$$

where δ_{ij} is the Kronecker symbol. If by $Q_{0ij} \neq 0$ we denote a particular component of the magnetic quadrupole tensor in the $\epsilon = 0$ limit, then as in the case of the magnetic moment, we conclude that Q_{1ij} is of $O(Q_{0ij})$ while Q_{2ij} is of $O(\epsilon Q_{0ij})$.

Using Eqs. (4) and (5) we can match the asymptotic behavior of solutions in regions $\mathbf{R}^3 \setminus \Omega$ and Ω. It is then possible to perturbatively obtain physical quantities to leading order in ϵ, using only the fields on Ω computed from the auxiliary problem. The fields and quantities evaluated from this problem are denoted by an overbar notation. We consider first the magnetic moment. On $\mathbf{R}^3 \setminus \Omega$, the scalar potential can be written as $\Phi = \Phi_a + \Phi_r$, where Φ_a is the potential due to the applied field and satisfies the open boundary condition at infinity, $-\nabla \Phi_a \to \mathbf{H}_a$, and Φ_r describes the presence of the superconductor. Since $\mathbf{m}_2$, as we have shown, explicitly scales with ϵ, it can be accurately computed to first order in ϵ by obtaining its leading contribution. This

is achieved by using the fields on Ω from the auxiliary problem, i.e., by writing $\bar{\Phi} = \Phi_a + \bar{\Phi}_r$. The task of determining $\mathbf{m}$ to $O(\epsilon m_0)$ is therefore reduced to that of correctly including the contribution of $\mathbf{m}_1$ to first order in ϵ. The exact solution for $\mathbf{H}$ is continuous on $\partial\Omega$. To calculate m_{1i}, the i-th component of $\mathbf{m}_1$, we can use the external fields obtained from Φ. The part of Φ_r which has a dipole character is characterized by the unknown vector $\mathbf{m}$, the correct value of the magnetic moment. The remaining part of Φ_r has different symmetry properties and does not contribute[7] to m_i. Contributions to the i-th component of $\mathbf{m}_1$, $i = x, y, z$, (we take $m_{0i} \neq 0$) can be written as

$$m_{1i}(\mathbf{m}) = m_{1i}(\Phi_a) + m_{1i}(\Phi_r), \tag{6}$$

where $m_{1i}(\Phi_a)$, for Φ_a, which is known, can be simply calculated from Eq. (4). We define p_{ij} by $m_{1i}(\Phi_a) \equiv \sum_j p_{ij} m_{0j}$, $i, j = x, y, x$. The constants p_{ij}, which depend on the shape of Ω, can now be determined by solving for p_{ij} using the known values $m_{1i}(\Phi_a)$ and m_{0i} corresponding to $\mathbf{H}_a$ applied along three independent directions. In the limit $\epsilon = 0$, $m_{2i} = 0$ and from Eq. (6) follows the identity

$$m_{0i} = \bar{m}_{1i} = \sum_j p_{ij} m_{0j} + \sum_j (\delta_{ij} - p_{ij}) m_{0j}, \tag{7}$$

where $m_{1i}(\bar{\Phi}_r) = \sum_j (\delta_{ij} - p_{ij}) m_{0j}$. For $\epsilon \neq 0$, when the solution for Φ and $\mathbf{H}$ is given in terms of a multipole expansion with unknown coefficients, $m_{1i}(\Phi_a)$ remains the same. The terms in Φ_r which contribute to the magnetic moment $\mathbf{m}$, will now have coefficients proportional to the correct unknown value of $\mathbf{m}$, slightly changed from the $\epsilon = 0$ case. We can therefore write $m_{1i}(\Phi_r) = \sum_j (\delta_{ij} - p_{ij}) m_j$ and the correct value for m_{1i} satisfies $m_{1i} = \sum_j [m_{ij} - p_{ij}(m_{ij} - m_{0ij})]$. Employing the fact that m_{2i} and $\bar{m}_{2i}$ agree to $O(\epsilon m_{0i})$ we can solve for m_i from $m_i = \sum_j [\delta_{ij} m_{ij} - p_{ij}(m_{ij} - m_{0ij})] + m_{2i}$, with the solution for m_i correct to $O(\epsilon)$,

$$m_i = m_{0i} + \sum_j p_{ij}^{-1} m_{2j} \approx m_{0i} + \sum_j p_{ij}^{-1} \bar{m}_{2j}. \tag{8}$$

Therefore the magnetic moment can be computed by only determining the lowest order contribution to $\mathbf{m}_2$.

Following an analogous procedure we can obtain a solution for the components of the quadrupole tensor Q_{ij} accurate to first order in ϵ. The resulting expression is similar to Eq. (8) with the constants p_{ij} replaced by the appropriate fourth rank tensor.

As a simpler example, it is instructive to consider an isotropic, linear superconducting sphere in an applied uniform magnetic field. Eq. (8) reduces[10] to the analytical result[5] $m = m_0(1 - 3\epsilon)$, where $m_0 = -H_a a^3/2$, $\epsilon \equiv \lambda/a$ and a is the sphere radius.

The ideas presented here can be used in problems in computational magnetics involving a small skin depth, by incorporating our perturbation procedure in the appropriate numerical algorithm. The integral identities for the magnetic multipoles are valid in the quasi-static regime and not restricted to the field of superconductivity.

We have addressed here the computation of small skin effects in a superconductor, using the perturbation method and matching the asymptotic behavior of a solution. We have shown how to accurately compute the nonlinear magnetic response of an anisotropic superconductor, by simplifying the boundary conditions and reducing the size of the computational domain.

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